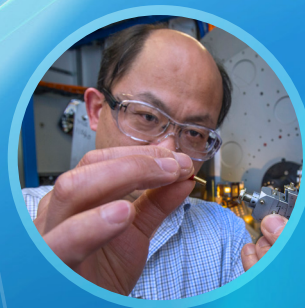


# *Exploring* **ENERGY** at BROOKHAVEN NATIONAL LABORATORY



U.S. DEPARTMENT OF  
**ENERGY**

Office of  
Science

**BROOKHAVEN**  
NATIONAL LABORATORY

# Exploring Energy

at BROOKHAVEN NATIONAL LABORATORY



*Brookhaven National Laboratory, a multipurpose research institution funded by the U.S. Department of Energy is a diverse resource for researchers seeking to tackle the grand challenges of energy storage and energy conversion. With our state-of-the-art facilities and wide network of partnerships, collaborators, and consortia across New York State, we combine professional expertise with advanced research tools.*

***Join us.***

# Exploring Energy

at BROOKHAVEN NATIONAL LABORATORY

*We are building and operating today's tools for tomorrow's discoveries.*

## Frontier Facilities

### Center for Functional Nanomaterials (CFN)

Modern nanoscience has enormous potential to develop solutions to our energy challenges as researchers strive to understand energy production, conversion, and storage at the nanoscale. Our

Center for Functional Nanomaterials has set out to fabricate and characterize novel nanomaterials, providing state-of-the-art facilities for researchers through a peer-reviewed system of access.



### National Synchrotron Light Source II (NSLS-II)

Researchers from all around the globe come for the brilliance of our x-rays and our state-of-the-art tools that enable frontier science and cutting-edge innovation. At the NSLS-II, we explore new energy materials by studying their structure, composition, chemistry, and physics, with the goal of designing better batteries and fuel cells.



### Interdisciplinary Science Building (ISB)

Our hub for energy research provides customized laboratories for multidisciplinary research teams embarking on the nation's most pressing energy and environmental quests. Our scientists undertake fundamental and applied studies to understand, engineer, and optimize materials with the goal of developing breakthrough technologies for batteries, biofuels, and solar panels.



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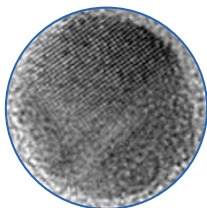
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## Multi-modal approach

*At Brookhaven Lab, we have the unique ability to study the structure, morphology, and chemistry of composite materials using a diverse set of techniques. By applying multiple techniques to a given problem, we can significantly enhance our understanding of these materials.*

*Our "multi-modal" approach helps us to solve the mysteries of novel materials and reveal their full potential for applications. By designing experiments to target specific studies and materials, we can use in-situ and in operando studies as well as a diverse range of experimental conditions to investigate materials and systems, pushing our knowledge to the next level.*

## Our Explorers' Tools



### X-ray Diffraction

We use state-of-the-art x-ray diffraction techniques to resolve the ordering and position of atoms or the size and shape of nanoparticles in new complex materials to fully understand their potential applications.



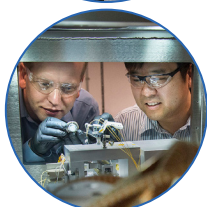
### X-ray Scattering

Our world-leading x-ray scattering tools offer the ability to reveal new insights about the crystal structure, chemical composition, and physical properties of complex materials and thin films.



### X-ray Spectroscopy

Using x-ray spectroscopy, we investigate the structural and chemical composition of materials such as batteries, catalysts, and fuel cells in real time, under real operating conditions (in operando).



### Imaging and Tomography

Using advanced x-ray imaging techniques in two and three dimensions, we investigate the complex composition of modern materials and map out the distribution of various elements within composite materials.



## Our Explorers' Tools

### Electron Microscopy

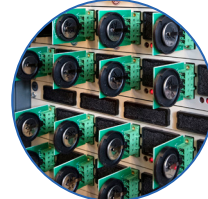
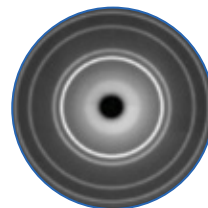
Electron microscopy offers a ten-million-times higher magnification than light microscopy, and we use it to “see” the nanostructures within battery composites and materials, and review their functional changes.

### Dry Room

We can fabricate and test prototype batteries like coin and pouch cells in a dry room, which is well-equipped with specialized research tools and controlled low humidity conditions.

### Computational Resources

Our Computational Science Initiative (CSI) provides one of the largest scientific data storage and analysis sites worldwide, combined with professional expertise in research, development, and deployment of novel methods and algorithms.



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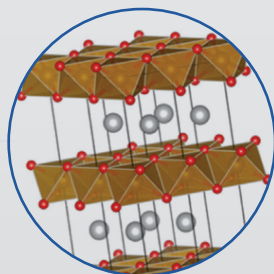
## Energetic Examples

*We share our research tools and expertise every day with researchers from industry, academia, and other institutions to tackle the most challenging questions about energy storage and energy conversion.*

## Battery Electrodes for the Future

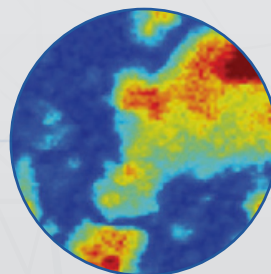
### Challenge

Rechargeable lithium-based batteries are used as lightweight power sources in many electronic devices, and silver ferrites are a promising new electrode material for designing improved batteries. Before these new materials can be used in future generations of batteries, their charging and discharging process—called lithiation/de-lithiation—needs to be characterized and analyzed. Researchers at Brookhaven National Laboratory and Stony Brook University studied a (de)lithiation process using ex-situ, in-situ and operando x-ray characterization techniques – including diffraction, spectroscopy, and imaging.



### Impact

These x-ray-based studies revealed a new atomic stacking order of the silver ferrite materials, which helped the researchers understand the potential of using silver ferrites as battery electrodes. Additionally, they were able to map the movement of the electrons during lithiation/de-lithiation, which gave them valuable information about the efficiency of the process.



(Left) Side-view of the AgFeO<sub>2</sub> layered structure showing the iron atoms in brown, silver atoms in silver, and oxygen atoms in red.

(Right) X-ray fluorescence nanoprobe image shows the iron distribution from in-situ cell studies.

Reference: J. L. Durham, A. B. Brady, C. A. Cama, D. C. Bock, C. J. Pelliccione, Q. Zhang, M. Ge, Y. R. Li, Y. Zhang, H. Yan, X. Huang, Y. Chu, E. S. Takeuchi, K. J. Takeuchi, A. C. Marschilok, *Phys. Chem. Chem. Phys.*, 19, 22329(2017), DOI: 10.1039/C7CP04012A.

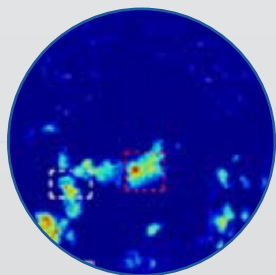
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## Battery 500 Consortium

### Challenge

If electric vehicles were affordable and convenient for all it would change the face of our towns and cities. For this to happen, these vehicles need a new generation of lithium batteries that can produce 500 watt-hours per kilogram, at a cost of less than \$100 per kilowatt-hour per battery pack. Scientists who design and synthesize new battery materials and systems need detailed understanding of the structure function relationship of these components.



### Impact

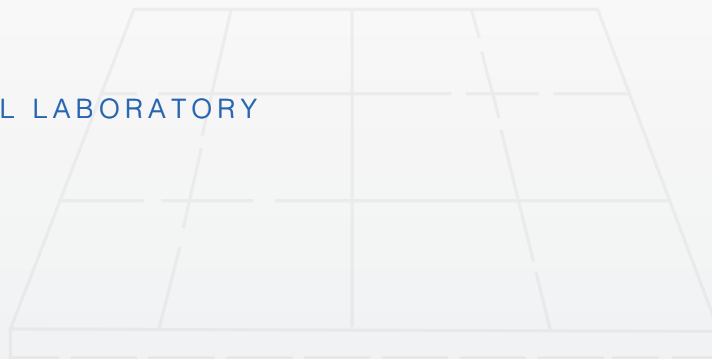
Brookhaven scientists are part of a multi-lab consortium sponsored by the DOE's Office of Energy Efficiency and Renewable Energy to work toward the goal of commercially-viable, next-generation batteries. Brookhaven Lab will focus on determining the characteristics of the composite solid electrolytes and sulfur cathodes using intense beams of x-rays at NSLS-II, mass-spectroscopy and high-resolution transmission electron microscopy at CFN, and other techniques available at Brookhaven's research facilities.



*(Left) Images of elemental distribution in solid-state electrolyte ceramic material collected at the hard x-ray nano-probe beamline at NSLS-II.*

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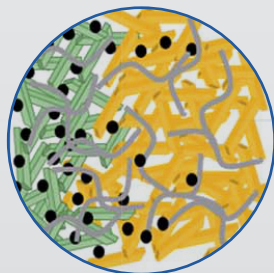
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## Understanding the discharge process within an intact battery

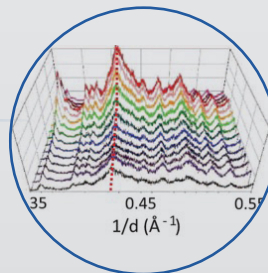
### Challenge

In order to operate at higher currents, most batteries require the addition of conductive additives such as carbon, which lowers the battery's volumetric energy density. In this case, the in situ formation of a silver matrix in a phosphate material transforms a material otherwise plagued by low conductivity. To optimize power output, the challenge is to determine where, when, and how these metallic silver networks are generated. This critical information about local phase evolution can only be obtained using the high flux of a synchrotron light source.



### Impact

Researchers at Stony Brook University and Brookhaven National Laboratory studied silver vanadium phosphates, which can generate these silver networks, and found a way to monitor the conductive silver metal framework it forms without destroying the batteries. The scientists employed a non-invasive, spatially resolved approach and investigated the battery during the discharge process under various conditions to determine what conditions will allow maximum utilization and power output from the battery.



(Left) Schematic diagram of the metallic silver networks.

(Right) In situ energy dispersive x-ray diffraction enabling visualization of the discharge progress.

References: K. Kirshenbaum, D. C. Bock, C.-Y. Lee, Z. Zhong, K. J. Takeuchi, A. C. Marschilok, E. S. Takeuchi. *Science*, 347(6218), 149 (2015). DOI: 10.1126/science.1257289

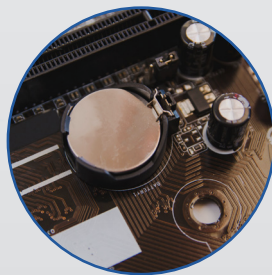
D.C. Bock, A.M. Bruck, C.J. Pelliccione, Y. Zhang, K. J. Takeuchi, A. C. Marschilok, E. S. Takeuchi, *RSC Advances*, 6, 106887 (2016). DOI: 10.1039/C6RA24024K





## Challenge

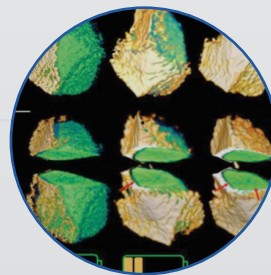
When charging a battery, a chemical phase transition from anisotropy (properties are varied through a material) to isotropy (properties are the same in all directions through a material) takes place, and this transition plays an essential role in determining the performance of a particular battery design. Understanding and tracking the evolution of these three-dimensional transformation features during the charging process is crucial for researchers to design the next generation of batteries.



## Charging revealed

### Impact

Scientists at Brookhaven's NSLS-II developed a novel x-ray technique using x-ray nano-imaging combined with x-ray spectroscopy to directly visualize and monitor the evolution of microstructures and chemical reactions within individual electrode micro particles. These insights into the phase transformation mechanism of batteries provide a better understanding of chemical reaction pathways and how they are correlated to battery performance, and will lead to better designs of advanced battery materials.



*(Left) Batteries are used in everyday life.*

*(Right) The chemical phase within the battery evolves as the charging time increases.*

Reference: J. Wang, Y. K. Chen-Wiegart, C. Eng, Q. Shen, J. Wang, *Nature Communications* 7,12372 (2016).

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## Working with Us

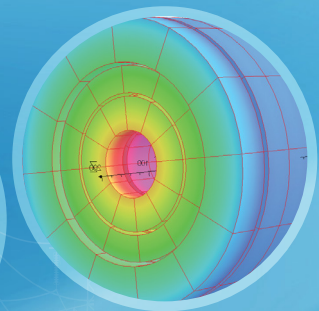
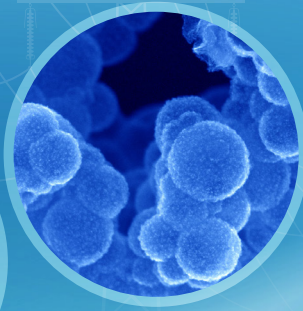
Brookhaven National Laboratory is an advanced international research and development campus and home to world-leading experts and state-of-the art facilities.

Brookhaven actively seeks partners to license its technologies and collaborate in multi disciplinary teams to accelerate innovation and development.

Small businesses are encouraged to explore potential research collaborations and technology development with us. Research collaborations with Brookhaven Lab can greatly strengthen small business innovation research (SBIR) and small business technology transfer (STTR) proposals and other federal- or state-funded programs.

A range of contracting mechanisms are available to facilitate working with us, from collaborative research agreements, to strategic partnership agreements, to user facility agreements.





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